6.4 BAND GAP : CONDUCTORS, SEMICONDUCTORS AND INSULATORS

Let us calculate the effective number of free electrons in a band so as to differentiate between conductors, insulators and semiconductors on the basis of band gap. We know that the electron in k-state is actually bounded to a lattice and therefore the effective mass of the electron is different from free electron mass.

Let us consider an empty band which is filled with electrons upto wave vector k_1 within the first Brillouin zone shown in Fig. 6.10. Here $k_1 < \frac{\pi}{a}$. The ratio of free electron mass to its effective mass in k-state can be taken as the extent to which an electron in that k state is free to take part in conduction.

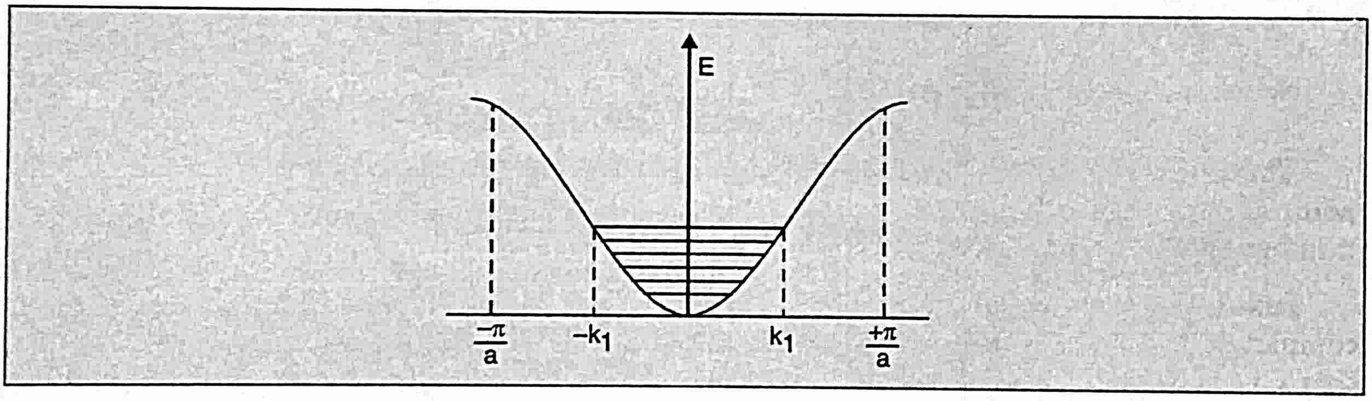

Fig. 6.10

i.e.

$$f_k = \frac{m}{m_{eff}} = \frac{m}{\hbar^2}\frac{d^2E}{dk^2}$$

Now in one dimension lattice of length L, the number of states in the interval dk is given by

$$dn = \frac{L}{2\pi}\,dk$$

Therefore, the effective number of electrons in interval dk is,

$$dN_{eff} = 2f_k\,\frac{L}{2\pi}\,dk$$

The factor 2 is due to Pauli's exclusion principle which states that each state is filled by

two electrons. Hence, integrating dN_{eff}, we get the total number of effective electrons if the band is filled upto k_1 is

$$N_{eff} = 2\int_{-k_1}^{+k_1} f_k \frac{L}{\pi}\, dk = \frac{2Lm}{\pi\hbar^2}\left(\frac{dE}{dk}\right)_{k=k_1}$$

Hence, the effective number of electrons available for conduction depends on the (dE/dk).

Band Gap : The difference between the highest value of energy in a given band and the lowest value of energy in the very next band above it is called the band gap. Band gaps are also called forbidden energy states.

The allowed energy bands in a solid at lowest temperature *i.e.* $0K$, lowest energy are filled with the available electrons from the bottom upwards, as per Pauli's exclusion principle, till all the electrons are accommodated. With the increase of temperature, the electrons in the valence band shift to still higher empty levels in the conduction band. The application of electric field or magnetic field also compels the electrons to cross the band gap and shift to conduction band. All solids do not behave alike. So some solids are classified conductors, some insulators and some are referred as semiconductors.

For a completely filled band, for example at the first Brillouin zone boundaries, $k = \pm\frac{\pi}{a}$, the slope of the curve in Fig. 6.10 is zero, as the graph is flat at the top.

So when $\frac{dE}{dk} = 0$, then $N_{eff} = 0$.

This means that the number of free electrons in a completely filled band is zero. The point at which the band is filled upto $k = k_0$ is called inflexion point. At this point the effective number of electrons becomes maximum.

Point to Remember

At inflexion point, the nature of slope, in the graph between *E* and *k*, changes sign from positive to negative.

1. Insulators

In insulators, the valence band is full while the conduction band is empty. They have a large energy gap between valence band and conduction band which is of the order of 5 eV to 15 eV. The energy band diagram is shown in fig. (7). They do not have any free electrons.

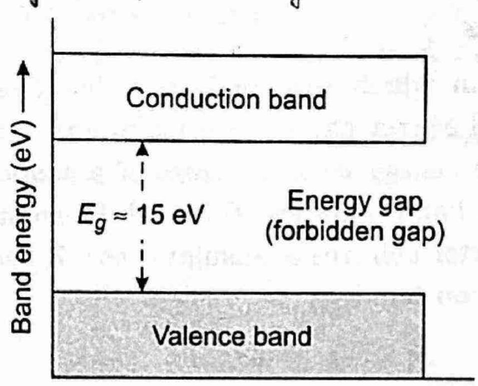

Fig. 7. Energy band diagram of insulator.

At room temperature, the valence electrons do not have much energy to jump from valence band to conduction band. So, they do not conduct electricity. Therefore, they have very high resistivity of the order of 10^9 Ω cm.

At very high temperature or under very high electric field, some electrons may move from valence band to conduction band. Hence, insulator may show small conductivity under above conditions.

The examples are : glass, diamond, etc.

diamond is a material whose covalent bond splits $2s$ and $2p$ levels into two band separated by an energy gap of $\Delta E_g = 6\, eV$ with the valence electrons filling the lower band and so diamond is an insulator.

2. Conductors

Conductors are the materials in which the conduction band and valence band overlap as shown in fig. (8). Alternatively, we can say that there is no energy gap or forbidden energy gap between valence band and conduction band.

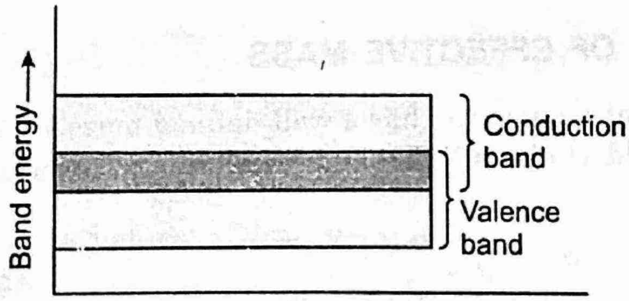

Fig. 8. Energy band diagram of conductor.

The conductors have large number of free electrons for electrical conduction. There is a single energy band called conduction band. This band is partially filled at any temperature.

As there is no energy gap, there is no structure to establish hole. When a small potential difference is applied across a conductor, the free electrons constitute the electric current. Due to this fact, a metal works as a very good conductor.

The examples are : Copper, aluminium, etc.

On the application of external field in any form such as electric, heat etc., electrons shifts from valence band to the conduction band, so these type of solids are called conductors. Even if there is a small energy gap as shown in fig. 6.11 (c), materials such as *Li, Na, K* etc. exhibit the conductivity. In the case of materials such as *Ba, Cd, Zn* etc. the valence band is completely filled and the empty conduction band overlaps the valence band. The electrons freely move inside the crystal lattice and cause conduction.

3. Semiconductors

The material in which the conduction band and valence band are separated by a small energy gap (1.1 eV for Si and 0.7 eV for Ge) are called semiconductors. The energy band diagram of a semiconductor is shown in fig. (9). The valence band is almost filled while conduction band is almost empty. A semiconductor behaves as insulator at 0 K because no electrons are available in conduction band.

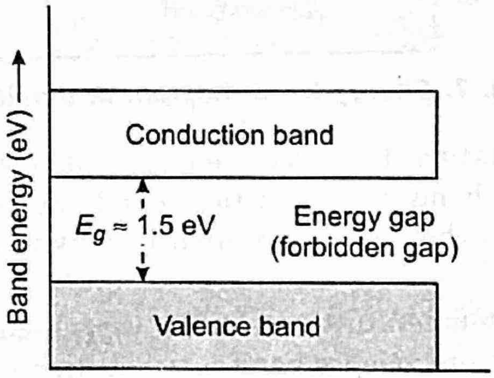

Fig. 9. Energy band diagram for a semiconductor.

When the temperature is increased, the forbidden band (energy gap) is decreased so that some electrons are liberated into conduction band. Similarly, a small electric field is required to push the electrons from valence band to conduction band. The conductivities are of the order of 10^2 mho-metre.

Examples are : Germanium, silicon, etc.

Conclusions :

(i) If the valence electrons exactly fill one or more bands, leaving other empty, the crystal is an insulator [Fig. 6.11(*a*)].

(ii) If the bands overlap, then instead of one filled band and the other over it fully empty, giving an insulator, we can have two partly filled bands giving a metal.

(iii) If the energy gap is very small ($E_g \simeq 0.025\ eV$) at room temperature, the electrons can rise from valence band to the conduction band on the application of field. Band overlap with some gap as in Fig. 6.11 (*c*), the crystals are called semi metals. Bismuth is an example of semi-metal.

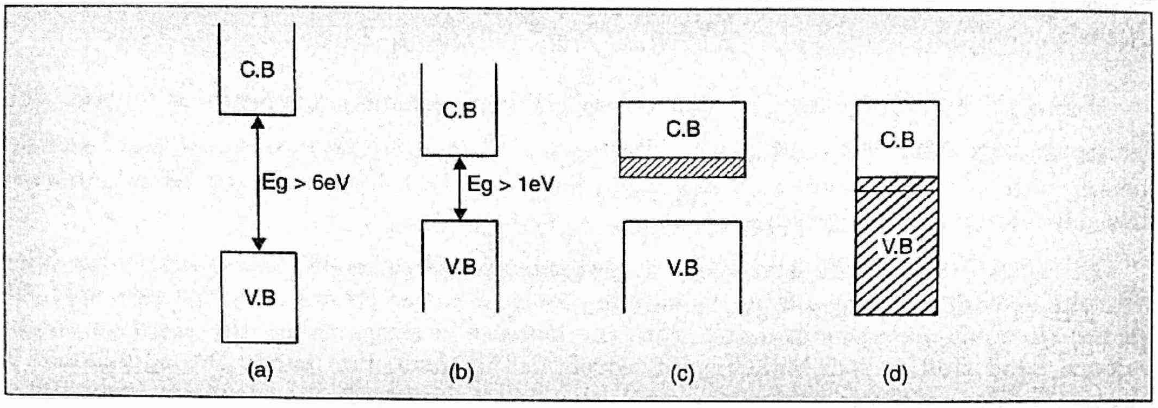

Fig. 6.11

5.6 CONCEPT OF HOLE

The concept of effective mass has a physical significance. We have seen that beyond the inflection points, the effective mass m^* becomes negative (see fig. 10). This is the region close to the top of the band. In this region, the velocity of electron decreases, *i.e.*, the acceleration is negative [fig. (11)]. This means that in this region of k-space, the lattice exerts a large retarding force on the electron which overcomes the applied force. Therefore, in the upper half of the band, the electron behaves as a positively charged particle referred to as a hole. The concept of hole provides a satisfactory description of charge carriers in the crystal.

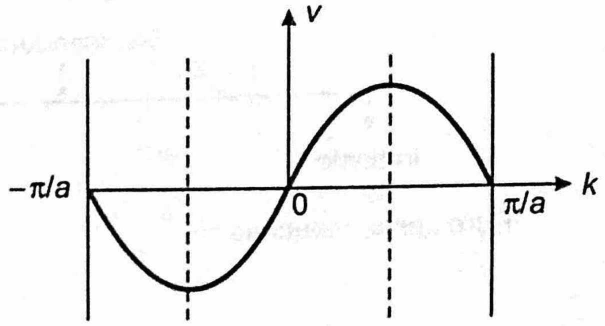

Fig. 11. Variation of *v* with *k*.

5.7 COMPARISON OF CONDUCTORS, INSULATORS AND SEMICONDUCTORS

Table : Comparison of conductors, insulators and semiconductors

S.No	Parameter	Conductors	Insulators	Semiconductors
1.	Conductivity	Very high	Very low	Moderate
2.	Resistivity	Very low	Very high	Moderate
3.	Forbidden gap	No forbidden gap	Large gap (> 3 eV)	Medium ($E_g = 1$ to 2 eV)
4.	Temperature coefficient of resistance	Positive	Negative	Negative
5.	Number of electrons available for conduction	Very large	Very small	Moderate
6.	Conductivity at room temperature	Very good	Poor	Moderate
7.	Examples	Aluminium, copper	Paper, mica, glass	Silicon, germanium
8.	Applications	As conductors, wires, bus bars	Capacitors, insulation for wires	Semiconductor devices